

Calculation of the divergence rate

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An abbreviated version of this protocol was published in eLIFE in Sep 2019

Molecular function limits divergent protein evolution on planetary timescales

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Detailed protocol

Inferring the divergence rate between orthologs as a function of divergence time or protein distance

1. Define t and y vectors to fit divergence model. For each pair of orthologs, values in t are the divergence time between species expressed in billions of years, values in y are the percent sequence identity between corresponding orthologs.
2. Use the `fitnlm` function in matlab (or an alternative nonlinear regression method) to fit equation 3 from Konaté *et al.* and retrieve the values for the R_0 and α parameters. (relevant matlab code shown below).

$$y = 100 * \left(\frac{R_0 * t}{\alpha} + 1 \right)^{-\alpha}$$

```
model3=@(b,x)100.*((b(1).*x/b(2))+1).^b(2)
beta=[1,0.5];
fit=fitnlm(t,y,model3,beta);
[R0,alpha]=fit.Coefficients.Estimate;
```

3. Use the obtained R_0 and α parameters in equation 5 from Konaté *et al.* to determine the divergence rate (dy/dt) at an arbitrary t expressed in billions of years.

$$\frac{dy}{dt} = -100 * R_0 \left(\frac{R_0 * t}{\alpha} + 1 \right)^{-\alpha-1}$$

4. Alternatively, use the obtained R_0 and α parameters in equation 4 from Konaté *et al.* to determine the divergence rate an arbitrary protein distance expressed as a fraction (i.e. 1 – percent identity/100)

$$\frac{\partial D}{\partial t} = R_0 * (1 - D)^{(\alpha+1)/\alpha}$$

How to cite: (Readers should cite both the Bio-protocol preprint and the original research article where this protocol was used)

1. Plata, G. (2021). Calculation of the divergence rate. Bio-protocol Preprint. bio-protocol.org/prep758.
2. Konaté, M. M., Plata, G., Park, J., Usmanova, D. R., Wang, H. and Vitkup, D. (2019). Molecular function limits divergent protein evolution on planetary timescales. eLIFE. DOI: [10.7554/eLife.39705](https://doi.org/10.7554/eLife.39705)

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